

Draft Risk Evaluation for 1,4-Dioxane
Draft Supplemental File:
Consumer Exposure Assessment
Model Input Parameters

November 2020

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Weight Fractions

Description
This tab provides the model inputs required to evaluate the presented consumer conditions of use (COU) using EPA's Consumer Exposure Model (CEM 2.1).
This tab provides the model inputs required to evaluate the inhalation pathway for the spray polyurethane foam (SPF) COU using EPA's Multi-Chamber Concentration and Exposure Model (MCCCEM).
This tab provides the identified weight fractions and sources for all evaluated product scenarios.

Parameter	Units
Chemical of Interest	n/a
CAS Number	n/a
CEM Model Scenario	n/a
Selected CEM Model Scenario - Dermal	n/a
Product User (s)	n/a
Activity Pattern	n/a
Product/Article Environment of Use	n/a
Background Concentration	mg/m ³
Select Pathways Evaluated in CEM	n/a
Modeling Options - Inhalation	n/a
Vapor Pressure (Lewis, 2010)	torr
Molecular Weight (Howard, 1990)	g/mol
Chemical Saturation Concentration in Air	mg/m ³
Log Octanol-Water Partition Coefficient (Hansch et al., 1995)	n/a
Water Solubility (Yalkowsky et al., 2010)	mg/mL
Gas Phase Mass Transfer Coefficient (CEM Estimate)	m/hr
Henry's Law Coefficient	atm/M
Emission Factor	ug/m ² /hr
Frequency of Use (Acute)	events/day
Frequency of Use (Chronic)	days/year
Product Density	g/cm ³
Film Thickness on Skin	cm
Product Dilution Factor	unitless
Maximum Weight Fraction	fraction
Mean Weight Fraction	fraction
Duration of Use Event - High-End, Inhalation	min/events
Duration of Use Event - Central Tendency, Inhalation	min/events
Duration of Use Event - High-End, Dermal	min/events
Duration of Use Event - Central Tendency, Dermal	min/events
Mass Used - High-End	g/event
Mass Used - Central Tendency	g/event
Fraction Product Ingested	n/a
Amount Retained on Skin	cm/hr
Skin Permeability Coefficient (Kp)	cm/hr
Absorption Fraction High-End Dermal Duration	n/a

Surface Cleaner	Antifreeze
1,4-Dioxane	1,4-Dioxane
123-91-1	123-91-1
Generic Product E1 (Emission from Product Applied to a Surface Indoors Incremental Source Model)	Generic Product E1 (Emission from Product Applied to a Surface Indoors Incremental Source Model)
Permeability (P DER2b)	Absorption Fraction (P DER2a)
Adult (Age ≥ 21) and Child (Age 11-20)	Adult (Age ≥ 21) and Child (Age 11-20)
User stays at home entire day	User stays at home entire day
Bathroom	Garage
0	0
Inhalation and Dermal	Inhalation and Dermal
E1, Let CEM Estimate Emission Rate, P_INH2, Emission Factor Method	E1, Let CEM Estimate Emission Rate, P_INH2, Use Emission Factor Method
40	40
88.1	88.1
1.89E+05	1.89E+05
-0.27	-0.27
800	800
3.2	3.2
n/a	n/a
0 (Chinn method)	0 (Chinn method)
Fixed at 1 event/day (CEM default)	Fixed at 1 event/day (CEM default)
365 (CEM high-end default); 300 (CEM central-tendency default)	n/a ²
1.09 (CEM scenario default)	1.12 (CEM scenario default)
0.00214 (CEM scenario default)	0.00655 (Recommended film thickness from Exposure Factors Handbook Table 7-2, based on immersion on ethanol and water)
Fixed at 1 (i.e., no dilution)	Fixed at 1 (i.e., no dilution)
9.00E-06	8.60E-05
n/a (unable to estimate mean from available sources)	n/a ²
30 (High-end scenario duration from CEM)	15 (High-end scenario duration from CEM)
15 (Central tendency duration from Westat survey)	n/a ²
30 (High-end scenario duration from CEM)	15 (High-end scenario duration from CEM)
15 (Central tendency duration from Westat survey)	n/a ²
300 (High-end scenario duration from CEM)	150 (High-end scenario mass from CEM)
200 (Central tendency scenario duration from CEM)	n/a ²
0.00E+00	0
n/a	1.12E-4 (CEM Estimate)
5.05E-4 (IHSkinPerm)	5.05E-4 (IHSkinPerm)
3.21E-01	2.62E-01 (CEM Estimate)

Dish Soap	Dishwasher Detergent
1,4-Dioxane	1,4-Dioxane
123-91-1	123-91-1
Generic Product E4 (Emission from Product Added to Water)	Generic Product E4 (Emission from Product Added to Water)
Permeability (P DER2b)	Absorption Fraction (P DER2a)
Adult (Age \geq 21) and Child (Age 11-20)	Adult (Age \geq 21) and Child (Age 11-20)
User stays at home entire day	User stays at home entire day
Kitchen	Kitchen
0	0
Inhalation and Dermal	Inhalation and Dermal
E4, Let CEM Estimate Emission Rate, P_INH2	E4, Let CEM Estimate Emission Rate, P_INH2
40	40
88.1	88.1
1.89E+05	1.89E+05
-0.27	-0.27
800	800
3.2	3.2
n/a	n/a
n/a	n/a
Fixed at 1 event/day (CEM default)	Fixed at 1 event/day (CEM default)
365 (CEM high-end default); 300 (CEM central-tendency default)	365 (CEM high-end default); 300 (CEM central-tendency default)
1.03 (CEM scenario default)	1.077 (CEM scenario default)
0.00655 (Recommended film thickness from Exposure Factors Handbook Table 7-2, based on immersion on ethanol and water)	0.00655 (Recommended film thickness from Exposure Factors Handbook Table 7-2, based on immersion on ethanol and water)
0.007 (estimated assuming high-end mass of product use [28g/use] in one gallon of water)	Fixed at 1 (i.e., no dilution)
2.04E-04	9.70E-06
2.40E-05	5.00E-06
20 (High-end scenario duration from CEM)	50 (High-end scenario duration from CEM)
10 (Central tendency scenario duration from CEM)	45 (Central tendency scenario duration from CEM)
20 (High-end scenario duration from CEM)	1 ⁴
10 (Central tendency scenario duration from CEM)	1 ⁴
84 (High-end of range from American Cleaning Institute Exposure and Risk Screening Methods for Consumer Product Ingredients ⁶ , which reported 28 g/use, up to three times per day)	40 (High-end scenario mass from CEM)
48 (Central tendency from American Cleaning Institute Exposure and Risk Screening Methods for Consumer Product Ingredients ⁶ , with a mean of 16 g/use, up to three times per day)	20 (Central tendency scenario mass from CEM)
0	0
n/a	1.08E-4 (CEM Estimate)
5.05E-4 (IHSkinPerm)	5.05E-4 (IHSkinPerm)
2.92E-01	3.77E-02

Laundry Detergent	Paint and Floor Lacquer
1,4-Dioxane	1,4-Dioxane
123-91-1	123-91-1
Generic Product E4 (Emission from Product Added to Water)	Generic Product E2 (Emission from Product Applied to a Surface Indoors Double Exponential Model)
Permeability (P DER2b)	Absorption Fraction (P DER2a)
Adult (Age ≥ 21) and Child (Age 11-20)	Adult (Age ≥ 21) and Child (Age 11-20)
User stays at home entire day	User stays at home entire day
Utility Room	Bedroom
0	0
Inhalation and Dermal	Inhalation and Dermal
E4, Let CEM Estimate Emission Rate, P_INH2	E2, Let CEM Estimate Emission Rate, P_INH2
40	40
88.1	88.1
1.89E+05	1.89E+05
-0.27	-0.27
800	800
3.2	3.2
n/a	n/a
n/a	n/a
Fixed at 1 event/day (CEM default)	Fixed at 1 event/day (CEM default)
365 (CEM high-end default); 300 (CEM central-tendency default)	n/a ²
1.03 (CEM scenario default)	1.25 (CEM scenario default)
0.00655 (Recommended film thickness from Exposure Factors Handbook Table 7-2, based on immersion on ethanol and water)	0.00981 (CEM scenario default)
0.016 (estimated assuming high-end mass of product used [60g] in one gallon of water)	1 (i.e., no dilution)
1.40E-05	3.00E-05
6.00E-06	n/a ²
50 (High-end scenario duration from CEM)	810 (95th percentile duration from Westat survey)
45 (Central tendency scenario duration from CEM)	n/a ²
20 (Central tendency scenario durations from CEM) ⁵	810 (95th percentile duration from Westat survey)
10 (Central tendency scenario durations from CEM) ⁵	n/a ²
60 (High-end scenario mass from CEM)	26025 (95th percentile, Westat Survey)
40 (Central tendency mass from CEM)	n/a ²
0	0
n/a	1.23E-2 (CEM Estimate)
5.05E-4 (IHSkinPerm)	5.05E-4 (IHSkinPerm)
2.92E-01	3.38E-01

Textile Dye	SPF (Dermal)
1,4-Dioxane	1,4-Dioxane
123-91-1	123-91-1
Generic Product E4 (Emission from Product Added to Water)	n/a ¹
Permeability (P DER2b)	Absorption Fraction (P DER2a)
Adult (Age ≥ 21) and Child (Age 11-20)	Adult (Age ≥ 21) and Child (Age 11-20)
User stays at home entire day	n/a ¹
Utility Room	n/a ¹
0	n/a ¹
Inhalation and Dermal	Dermal
E4, Let CEM Estimate Emission Rate, P_INH2	n/a ¹
40	40
88.1	88.1
1.89E+05	1.89E+05
-0.27	-0.27
800	800
3.2	3.2
n/a	n/a
n/a	n/a
Fixed at 1 event/day (CEM default)	Fixed at 1 event/day (CEM default)
n/a ²	n/a ²
0.65 (CEM scenario default)	0.0384 (based on density of typical closed cell, medium density SPF, with densities ranging from 1.5 - 2.4 lbs/ft ³) ACC, 2016
0.00655 (Recommended film thickness from Exposure Factors Handbook Table 7-2, based on immersion on ethanol and water)	0.01 (CEM default)
0.1	1 (i.e., no dilution)
4.70E-06	5.00E-04
n/a ²	n/a ²
20 (High-end scenario duration from CEM)	360 (basement, attic); 180 (garage)
n/a ²	n/a ²
20 (High-end scenario duration from CEM)	360 (basement, attic); 180 (garage)
n/a ²	n/a ²
100 (High-end scenario duration from CEM)	n/a ¹
n/a ²	n/a ²
0	0
n/a	0.000384
5.05E-4 (IHSkinPerm)	5.05E-4 (IHSkinPerm)
2.92E-01	3.38E-01

Absorption Fraction Central Tendency Dermal Duration ³	n/a
Surface Area-Body Weight (SA-BW) Adult	cm ² /kg
Surface Area-Body Weight (SA-BW) Adult 16-20	cm ² /kg
Surface Area-Body Weight (SA-BW) Child 11-15	cm ² /kg
Building Volume (Residence)	m ³
Use Environment Volume	m ³
Near Field/Far Field Volume	m ³
Air Exchange Rate, Zone 1 (Residence)	hr ⁻¹
Air Exchange Rate, Zone 2 (Residence)	hr ⁻¹
Interzone Ventilation Rate	m ³ /hr
Air Exchange Rate, Near-Field Boundary	hr ⁻¹
Use Start Time	n/a

¹ Inhalation exposures for the SPF scenario were evaluated using MCCCEM with

² Chronic exposures not evaluated for scenarios that are expected to involve in

³ For scenarios where chronic exposures are evaluated, central tendency duration

⁴ The exposure duration applied for dermal exposures to dishwashing detergent

⁵ The exposure duration applied for dermal exposures to laundry detergent was

⁶ https://www.aciscience.org/docs/Consumer_Product_Ingredient_Safety_v2.0.

2.62E-01	n/a ²
3.10 (CEM default mean, inside of one hand)	3.10 (CEM default mean, inside one hand)
2.90 (CEM default mean, inside of one hand)	2.90 (CEM default mean, inside one hand)
3.17 (CEM default mean, inside of one hand)	3.17 (CEM default mean, inside one hand)
492	492
15	90
1/14	1/89
0.45 (CEM default)	0.45 (CEM default)
0.45 (CEM default)	0.45 (CEM default)
107 (Koontz and Rector, 1995)	107 (Koontz and Rector, 1995)
402 (CEM default)	402 (CEM default)
9:00 AM	9:00 AM

h measured emission data, please see other tab for relevant inputs.

frequent and or intermittent use frequencies.

ons of exposure were applied to dermal estimates, which impacts the estimation of absorption fraction within P_DER2
t were adjusted/lowered to 1 minute, as the scenario default exposure duration is based on the run time of a dishwashe
e adjusted/lowered to be equal to the default exposures times for hand dish soap, as this dermal exposure scenario is in
.pdf

2.14E-01	3.77E-02
12.4 (CEM default mean, both hands)	1.24 (CEM default mean, 10% of hands)
11.6 (CEM default mean, both hands)	1.16 (CEM default mean, 10% of hands)
12.7 (CEM default mean, both hands)	1.27 (CEM default mean, 10% of hands)
492	492
24	24
1/23	1/23
0.45 (CEM default)	0.45 (CEM default)
0.45 (CEM default)	0.45 (CEM default)
107 (Koontz and Rector, 1995)	107 (Koontz and Rector, 1995)
402 (CEM default)	402 (CEM default)
9:00 AM	9:00 AM

2a.

r, not on expected dermal contact time.

ntended to approximate dermal contact from hand washing of clothing, whereas the default exposure durations for the lau

2.14E-01	n/a ²
12.4 (CEM default mean, both hands)	15.8 (CEM default mean, face, hands, and arms)
11.6 (CEM default mean, both hands)	14.9 (CEM default mean, face, hands, and arms)
12.7 (CEM default mean, both hands)	16.4 (CEM default mean, face, hands, and arms)
492	492
20	36
1/19	1/35
0.45 (CEM default)	0.45 (CEM default)
0.45 (CEM default)	0.45 (CEM default)
107 (Koontz and Rector, 1995)	107 (Koontz and Rector, 1995)
402 (CEM default)	402 (CEM default)
9:00 AM	9:00 AM

ndry detergent scenario are based on run times of the washing machine.

n/a ²	n/a ²
12.4 (CEM default mean, both hands)	15.8 (CEM default mean, face, hands, and arms)
11.6 (CEM default mean, both hands)	14.9 (CEM default mean, face, hands, and arms)
12.7 (CEM default mean, both hands)	16.4 (CEM default mean, face, hands, and arms)
492	n/a ¹
20	n/a ¹
1/19	n/a ¹
0.45 (CEM default)	n/a ¹
0.45 (CEM default)	n/a ¹
107 (Koontz and Rector, 1995)	n/a ¹
402 (CEM default)	n/a ¹
9:00 AM	n/a ¹

Parameter	Units	Exposure Scenario		
		Attic	Basement	Garage
Model Start Time	day/hour/min	0/0/0	0/0/0	0/0/0
Length of Model Run	day/hour/min	10/0/0	10/0/0	10/0/0
Reporting Interval	day/hour/min	0/0/1	0/0/1	0/0/1
House Code	N/A	HY013	HY014	HY015
State	N/A	NA	NA	NA
Stories	N/A	2	2	2
Volume	m ³	615	492	610
Season	N/A	NA	NA	NA
Whole House ACH	1/hr	1.56	0.45	0.85
Number of Zones	N/A	2	2	2
Source Description	N/A	SPF	SPF	SPF
Start Time	day/hour/min	0/9/0	0/9/0	0/9/0
End Time	day/hour/min	0/15/0	0/15/0	0/12/0
Zone	N/A	1	1	1
Source Model	N/A	Incremental	Incremental	Incremental
Total Mass of Chemical Released	mg	4524	4528	2170
Percent of Mass Associated with First Exponential	%	100	100	100
First-Order Rate Constant (first exponential)	1/hour	0.1	0.1	0.1
First-Order Rate Constant (second exponential)	1/hour	0.1	0.1	0.1
Events per Year	1/year	0.1	0.1	0.1
Years of Exposure	years	57	57	57
Body Weight	kg	80	80	80
Length of Life	years	78	78	78

Attic Application Scenario

Zone Characteristics				
Zone Number	Description	Volume (m ³)	Total-Flow-In (m ³ /hr)	Total-Flow-Out (m ³ /hr)
1	Attic	123	799.50	799.50
2	ROH	492	282.90	282.90

Interzonal Air Flow Rate (m ³ /hr)				
To From	Zone 0	Zone 1	Zone 2	Zone 3
Zone 0	-	738	221.4	0
Zone 1	738	-	61.5	0
Zone 2	221.4	61.5	-	0
Zone 3	0	0	0	-
Zone 4	0	0	0	0

Activity Pattern(s)				
Primary User Days in Effect: 1 Bystander Days in Effect: 0	Zone Number	Enter Time (hr)	Enter Time (min)	Breathing Rate (m ³ /day)
	2	0	0	15.08
	1	9	0	15.08
	2	15	0	15.08
Secondary User Days in Effect: 2 - 7 Bystander Days in Effect: 1-7	Zone Number	Enter Time (hr)	Enter Time (min)	Breathing Rate (m ³ /day)
	2	0	0	15.08

Basement Application Scenario

Zone Characteristics				
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Zone 4
0
0
0
0
-

Zone Number	Description	Volume (m³)	Total-Flow-In (m³/hr)	Total-Flow-Out (m³/hr)
1	Basement	246	219.70	219.70
2	ROH	246	219.70	219.70

Interzonal Air Flow Rate (m³/hr)

To From	Zone 0	Zone 1	Zone 2	Zone 3
Zone 0	-	110.7	110.7	0
Zone 1	110.7	-	109	0
Zone 2	110.7	109	-	0
Zone 3	0	0	0	-
Zone 4	0	0	0	0

Activity Pattern(s)

Primary User Days in Effect: 1 Bystander Days in Effect: 0	Zone Number	Enter Time (hr)	Enter Time (min)	Breathing Rate (m³/day)
	2	0	0	15.08
	1	9	0	15.08
	2	15	0	15.08
Secondary User Days in Effect: 2 - 7 Bystander Days in Effect: 1-7	Zone Number	Enter Time (hr)	Enter Time (min)	Breathing Rate (m³/day)
	2	0	0	15.08

Garage Application Scenario

Zone Characteristics

Zone Number	Description	Volume (m³)	Total-Flow-In (m³/hr)	Total-Flow-Out (m³/hr)
1	Garage	118	404.00	404.00
2	ROH	492	330.40	330.40

Interzonal Air Flow Rate (m³/hr)

To From	Zone 0	Zone 1	Zone 2	Zone 3
Zone 0	-	295	221.4	0
Zone 1	295	-	109	0
Zone 2	221.4	109	-	0
Zone 3	0	0	0	-
Zone 4	0	0	0	0

Activity Pattern(s)

Primary User Days in Effect: 1 Bystander Days in Effect: 0	Zone Number	Enter Time (hr)	Enter Time (min)	Breathing Rate (m³/day)
	2	0	0	15.08
	1	9	0	15.08
	2	12	0	15.08
Secondary User Days in Effect: 2 - 7 Bystander Days in Effect: 1-7	Zone Number	Enter Time (hr)	Enter Time (min)	Breathing Rate (m³/day)
	2	0	0	15.08

Zone 4
0
0
0
0
-

Zone 4
0
0
0
0
-

Consumer Conditions of Use
Category
Paints and Coatings
Cleaning and Furniture Care Products
Laundry and Dishwashing Products
Laundry and Dishwashing Products
Laundry and Dishwashing Products
Arts, Crafts, and Hobby Materials
Other Consumer Uses
Automotive Care Products

¹ The select Safety Data Sheet may now be superseded by a more recent version or formulation.

	Reported Product Concentration (ppm)						
Subcategory	<u>Kwon et al., 2007</u>	<u>Fuh et al., 2005</u>	<u>Tanabe and Kawata, 2008</u>	<u>Tahara et al., 2013</u>	<u>OCA, 2009</u>	<u>Citizens Campaign for the Environment, 2018</u>	<u>Citizens Campaign for the Environment, 2019</u>
Paint or Floor Lacquer							
Surface Cleaner	9		0.36 - 1.2				
Dish Soap				4.79 - 7.15	0.7 - 204		2.5 - 7.7
Dishwasher Detergent		6.5	0.86 - 9.7				
Laundry Detergent			0.05 - 2.1			2 - 14	0.22 - 14
Textile Dye							
Spray Polyurethane Foam	<i>Based on concentration of mixed SPI</i>						
Antifreeze							

tions					Overall Range (ppm)	Mean (ppm)
<u>ACA, 2015 Public Comment Submission (EPA-HQ-OPPT- 2015-0078)</u>	<u>Sapphire Group Inc., 2007</u>	<u>Makino et al., 2006</u>	<u>Danish EPA, 2005</u>	<u>Peak Extended Life Antifreeze & Coolant (2002) Safety Data Sheet1</u>		
0.02 - 30					0.02 - 30	
					0.36 - 9	Cannot estimate - unknown number of products tested in Kwon et al., 2007
		51			0.7 - 204	24
					0.86 - 9.7	5
		< 25			0.05 - 14	6
			4.7		4.7	
⁷ used in the occupational exposure scenario						
	0.01 - 22			86	0.01 - 86	

Maximum Weight Fraction (%)	Maximum Weight Fraction Input	Mean Weight Fraction Input
0.003%	3.00E-05	
0.0009%	9.00E-06	n/a
0.0204%	2.04E-04	2.40E-05
0.00097%	9.70E-06	5.00E-06
0.0014%	1.40E-05	6.00E-06
0.00047%	4.70E-06	
0.05%	5.00E-04	
0.0086%	8.60E-05	